What simulations can teach us about homogeneous ice nucleation

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In the last 5 years we have been using computer simulations with the aim of shedding light in the process of ice nucleation. Such process is the first step of water freezing, arguably the liquid-to-solid transition with the greatest relevance on Earth. In particular, the extent of freezing in atmospheric clouds has a great impact on the Earth's albedo and, therefore, on climate change [1]. Simulations is a particularly suitable tool to study ice nucleation because it enables access to the time and length scales relevant to this process, ns and nm, complementing the information obtained in experiments where such small scales can not be probed.

In 2013 and 2014 we published a JACS [2] and a J. Chem. Phys. paper [3] respectively where we computed nucleation rates for homogeneous ice nucleation at normal pressure and for different water models. For the first time, we showed a quantitative agreement between experimental measures and simulation calculations. In 2015 we published a paper in J. Chem. Phys. where we studied the competition between ice Ih and ice Ic polymorphs in ice nucleation [4]. More recently, we have published a paper on Phys. Rev. Lett. dealing with the effect of pressure on the nucleation of ice I [5]. Kanno and Angel showed in a seminal work in 1975 that pressure slows down ice nucleation [6]. This unexplained experimental fact has been exploited to avoid the deleterious ice formation in the cryopreservation of biological samples [7]. In our recent work [5] we provide an explanation for the decelerating effect of pressure on ice nucleation. Even more recently, we have plublished a paper on J. Chem. Phys. [8] where we propose a tentative explanation for current discrepancies in measures of the homogeneous ice nucleation rate by different groups [9].

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